Particle-hole excitations in normal liquid ^{3}He

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The dynamic form factor $S(Q,E)$ in liquid ^{3}He is evaluated in the momentum-transfer range $2 \leq Q \leq 5$ Å^{-1} for comparison with neutron scattering measurements. In this momentum range the neutrons excite chiefly interacting single particle-hole (p-h) excitations but no collective excitations. $S(Q,E)$ is calculated within an extended random-phase approximation (RPA) and the single p-h energy spectrum and p-h interaction needed in the RPA is provided by the Galitskii-Feynman-Hartree-Fock (GFHF) theory of liquid ^{3}He. The GFHF is a first-principles theory having no adjustable parameters with only the pair interatomic potential as input. Comparison with experiment suggests that the excitations at $Q=2$ Å^{-1} are well described by a single p-h excitation spectrum having effective mass $m^* \approx 1$, a strongly negative spin-symmetric p-h interaction and a nearly zero spin-antisymmetric interaction. This comparison also suggests that the p-h spectrum is well represented by the GFHF spectrum, the real part of the interaction by the Galitskii-Feynman (GF) T matrix, but that the imaginary part of the GF T matrix is too large.

I. INTRODUCTION

Neutron scattering studies[1-4] have provided exciting new information on the collective and elementary excitations in normal liquid ^{3}He. These measurements observe a dynamic form factor $S(Q,E)$, which is a sum of scattering from the density excitations and from the spin-density excitations. At wave-vector transfers $Q \lesssim 1.5$ Å^{-1}, the observed dynamic form factor shows a two-peak structure. The peak at lower energy E is identified as a "paramagnon"-like resonance in the spin-density component, while the peak at higher energy is identified with the zero-sound mode in the density excitation extending up to $Q \sim k_F$.[5] At $Q \geq 1.5$ Å^{-1}, both peaks disappear and the observed $S(Q,E)$ is characteristic of scattering chiefly from interacting single quasiparticle-quasihole excitations in both components. To date, the measurements have been confined to $Q \lesssim 2.5$ Å^{-1}.

Several models[2,6-14] have been developed which describe the shape of $S(Q,E)$ well. The most successful is the polarization-potential theory of liquid helium developed by Aldrich and Pines[6] which provides a detailed description of $S(Q,E)$ for $Q \lesssim 2$ Å^{-1}. The interplay between this theory and experiment has led to the development of phenomenological polarization potentials which have been successfully used to describe quite independent properties,[15] such as transport coefficients[16] and the superfluid transition temperature.[17] At low Q, Glyde and Khanna[8,9] obtained good agreement with the observed $S(Q,E)$ using a simple quasiparticle-hole interaction that is a straightforward extension of Landau theory to finite Q and E. This extension was proposed by Babu and Brown.[18] Yoshida and Takeno,[11] with the use of the memory function method and astute use of sum rules, obtained essentially the same interaction as used by Glyde and Khanna and similar results for $S(Q,E)$. The spin-dependent part of the scattering does, however, seem best described by the simple paramagnon model employed by Beal-Monod,[13] using an effective mass $m^*=1$ and a single interaction parameter.

In this paper we present a calculation of $S(Q,E)$ at higher wave-vector transfer, $2 \leq Q \leq 5$ Å^{-1}. At these Q values we expect the neutrons to excite only single quasiparticle-hole excitations with a possible coupling to multiparticle-hole states via the quasiparticle interaction. To describe normal ^{3}He we use the Galitskii-Feynman-Hartree-Fock (GFHF) theory,[19] which has been applied to the ground-state properties of both normal[20] and fully spin-polarized ^{3}He.[21] This is a first-principles theory which has as input only the pair interatomic potential. In the present application the quasiparticle (hole) states will be approximated by the GFHF single-particle energies (SPE's) and the quasiparticle interaction by the GF T matrix. The aim is to explore $S(Q,E)$ at higher Q, and to test how well the GFHF theory describes the dynamics of ^{3}He at Q values where the liquid does not support collective excitations.

The $S(Q,E)$ to be calculated is related to the corresponding dynamic susceptibility $\chi(Q,E)$ by

$$S(Q,E) = -\frac{\Omega_0}{\pi}[n(E)+1]\,\mathrm{Im}\chi(Q,E)\,, \tag{1}$$

where $n(E)$ is the Bose function and Ω_0 is the volume per atom. Takeno and Yoshida[22] have shown that the full $\chi(Q,E)$ of a liquid, quantum or classical, can, quite generally, be expressed in the form

$$\chi(Q,E) = \frac{\chi^0(Q,E)}{1-\Gamma(Q,E)\chi^0(Q,E)}\,. \tag{2}$$

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This is the form used by Aldrich and Pines[6] and by Pathak and Lücke.[14] Here $\chi^0(Q,E)$ is the dynamic susceptibility of a reference system of noninteracting particles satisfying the same statistics as the liquid particles. All the interaction effects are incorporated in $\Gamma(Q,E)$, which is, in general, complex and includes moments of the memory function. Here, we represent χ^0 by the Lindhard function

$$\chi^0(Q,E)=\frac{1}{\Omega}\sum_k \frac{n(k)-n(k+Q)}{E-[\epsilon(k+Q)-\epsilon(k)]} , \tag{3}$$

with the $\epsilon(k)$ given by the GFHF single-particle energies. Our reference system is therefore a system of noninteracting fermions having complex Hartree-Fock energies. The interaction $\Gamma(Q,E)$ is represented by the GF T matrix which is also complex. Equation (2) reduces to the standard random-phase approximation (RPA) if the $\epsilon(k)$ are free-particle energies and $\Gamma(k)$ is the Fourier transform of the interatomic potential. Equations (2) and (3) can therefore be viewed as an extended RPA using HF energies and the bare interaction replaced by a T matrix. The broad aim of our work is to see how well $S(Q,E)$ is described using the GFHF $\epsilon(k)$ and the T matrix with a $\chi(Q,E)$ given by (2).

Why might the GF T matrix represent the full quasiparticle-quasihole (qp-qh) interaction $\Gamma(Q,E)$ well in the range $2\leq Q\leq 5$ Å^{-1}? Firstly, the full interaction is often separated into a direct and an induced part.[18] The induced part corresponds to the interaction between a qp-qh pair induced via the density and spin-density fluctuations. Since the liquid does not support observable density or spin-density excitations at $Q\geq 1.5$ Å^{-1}, we expect the induced component to be small at large Q. Secondly, the energy transfers at $Q\geq 2$ Å^{-1} are large, substantially larger than the depth of the attractive well of the pair potential (≈ -10 K). Thus the interacting quasiparticles should be chiefly affected by the steeply repulsive hard core of the potential with the attractive well playing a much smaller role. The direct interaction should therefore be predominately pair wise via the repulsive hard core of the potential, an interaction well described by a T matrix.

In the next section we outline the form of $S(Q,E)$ and the ingredients of the GFHF theory. The results are presented in Sec. III and discussed in Sec. IV.

II. THEORETICAL BACKGROUND

A. Dynamic form factor

The inelastic scattering cross section observed when neutrons scatter from liquid ^{3}He is proportional to[1,3,23]

$$S(Q,E)=S_c(Q,E)+\frac{\sigma_i}{\sigma_c}S_I(Q,E) . \tag{4}$$

Here, $\hbar Q(E)$ is the momentum (energy) transferred from the neutron to the liquid in the scattering, and $\sigma_c(\sigma_i)$ is the coherent (incoherent) scattering cross section. We use $\sigma_c=4.9$ b (Ref. 24) and the ratio $\sigma_i/\sigma_c=0.25$, which is consistent with direct measurements of σ_i and with the inelastic scattering results of Sköld and Pelizzari.[4] In (4),

$$S_c(Q,E)=\frac{1}{2\pi\hbar}\int dt\, e^{iEt/\hbar}\frac{1}{N}\langle\rho(Q,t)\rho(-Q,0)\rangle$$

is the usual coherent dynamic form factor depending upon the Fourier component $\rho(Q,t)$ of the particle density, and

$$S_I(Q,E)=\frac{1}{2\pi\hbar}\int dt\, e^{iEt/\hbar}\frac{1}{NI(I+1)} \times\langle\vec{I}(Q,t)\cdot\vec{I}(-Q,0)\rangle \tag{5}$$

is a spin-dependent counterpart depending upon the Fourier component,

$$\vec{I}(Q,t)=\sum_l \vec{I}_l e^{-i\vec{Q}\cdot\vec{r}_l(t)} ,$$

of the spin density. If the spins are independent, $S_I(Q,E)$ reduces to the usual incoherent dynamic form factor.

$S_c(Q,E)$ is related through (1) to the Fourier transform of a density dynamic susceptibility defined as

$$\chi_c(Q,t)=-i\frac{\Theta(t)}{\hbar\Omega}\langle[\rho(Q,t),\rho(-Q,0)]\rangle , \tag{6}$$

where $\Theta(t)$ is the Heaviside step function and [,] are the commutator square brackets. The $S_I(Q,E)$ is similarly related to a spin susceptibility,

$$\chi_I(Q,t)=-i\frac{\Theta(t)}{\hbar\Omega}\langle[I(Q,t),I(-Q,0)]\rangle . \tag{7}$$

The χ_c (χ_I) are in turn given by the general form (2) in terms of the spin-symmetric (spin-antisymmetric) interaction $\Gamma^s=\frac{1}{2}(\Gamma^{\uparrow\uparrow}+\Gamma^{\uparrow\downarrow})$ [$\Gamma^a=\frac{1}{2}(\Gamma^{\uparrow\uparrow}-\Gamma^{\uparrow\downarrow})$] as

$$\chi_{c,I}(Q,E)=\frac{\chi^0(Q,E)}{1-\Gamma^{s,a}(Q,E)\chi^0(Q,E)} , \tag{8}$$

where χ^0 is given by (3).

Clearly, if $\Gamma^s=\Gamma^a=0$, then both S_c and S_I reduce to the noninteracting Fermi particle form

$$S_0(Q,E)=-\frac{\Omega_0}{\pi}[n(E)+1]\,\mathrm{Im}\chi^0(Q,E) . \tag{9}$$

In this case, from (3), the incoming neutron excites a single particle in state $\epsilon(k)$ with the Fermi sea to a state $\epsilon(k+Q)$ above the Fermi sea. The neutron, which transfers a momentum $\hbar Q$ and energy E to the liquid, thereby creates a particle-hole pair having a momentum difference of $\hbar Q$ and an excited energy $E=\epsilon(k+Q)-\epsilon(k)$. As noted in the Introduction, the $\epsilon(k)$ is given here by the GFHF-SPE spectrum.

When the p-h interact, χ is given by (8), and here the interaction between the particle and hole is represented by the appropriate spin-dependent GF T matrix.

B. GFHF theory

The GFHF theory is developed in several texts,[19] and has been discussed in detail for liquid ^{3}He recently.[20,21] Briefly, it begins with N noninteracting ^{3}He atoms (fermions) in a box of volume Ω. Here, we set the density at the observed value of ^{3}He at saturated vapor pressure, $\Omega_0=36.83$ cm^3/mole. The interaction between the atoms

via the pair potential is then included to first order. This leads to the Hartree-Fock approximation. The interaction between pairs via the pair potential is then summed to all orders. This summation is formally effected by replacing the Fourier transform of the pair potential by a complex and energy-dependent T matrix leading to the GFHF approximation. The GF T matrix depends upon the HF SPE $\epsilon(k)$, and $\epsilon(k)$ depends upon the T matrix. The T matrix and $\epsilon(k)$ must therefore be evaluated iteratively until consistent. After the iteration, we renormalized the self-consistent T matrix by z_k^2, where $z_k=[1-\partial\epsilon(k,E)/\partial E]^{-1}$ is the residue of the single-particle Green function at the quasiparticle pole. In liquid ^{3}He we found[20] $z_k\approx 0.6$ independent of k in the range $1\leq k\leq 2.5$ Å^{-1} of interest here. The renormalized $z_k^2\Gamma^{s,a}(Q,E)$ should be the most appropriate interaction to use with a Hartree-Fock-like χ^0.

For the pair potential we have used interchangeably the Beck[25] and HFDHE2 potential of Aziz *et al.*[26] For the present $S(Q,E)$ there is no significant difference between the two, although the GFHF ground-state energy of spin-polarized ^{3}He is lower by ~ 0.2 K using the Aziz *et al.* potential.

In general the T matrix, $\Gamma(k_{12},k_{34},P;E)$, depends upon the relative incoming momentum of the interacting pair $k_{12}=\frac{1}{2}(\vec{k}_1-\vec{k}_2)$, the relative outgoing momentum of the pair $k_{34}=\frac{1}{2}(\vec{k}_3-\vec{k}_4)$, and the c.m. momentum $P=\frac{1}{2}(\vec{k}_1+\vec{k}_2)$. In an RPA-like form (2), the relative incoming and outgoing momenta are the same, $k_{34}=k_{12}$. Also, $Q=k_1-k_2=2k_{12}$ is the momentum difference of the interacting qp-qh pair. We chose $P=0$ rather arbitrarily. The $\Gamma^{s,a}$ in (8) then reduces to $\Gamma(Q,E)$ with $Q=2k_{12}$.

III. RESULTS

The GFHF single-particle energy (SPE) spectrum $\epsilon(k)$ is shown in Fig. 1. This is the final $\epsilon(k)$ obtained by iterating the GF T matrix and $\epsilon(k)$ until consistent. This $\epsilon(k)$ gives a ground-state energy of -3.1 K at $\Omega_0=36.83$ cm^3/mole. In Fig. 1 we see that the Re$\epsilon(k)$ is shifted downward, due to the net attractive interaction between the atoms, from the original noninteracting kinetic energy, $\epsilon^0(k)=\hbar^2k^2/2M$. The real Re$\epsilon(k)$, however, has the same general dependence on k as $\epsilon^0(k)$, except for the constant shift to lower energy and has an effective mass of $m^*\approx 1$, independent of k. Thus we expect the difference $\epsilon(k+Q)-\epsilon(k)$ appearing in χ^0 to be approximately the same for Re$\epsilon(k)$ as for $\epsilon^0(k)$. The $\epsilon(k)$ has, however, an imaginary part which we expect to spread χ^0 over a wider energy range.

In Fig. 2 we show $\chi^0(Q,E)$ at $Q=2$ Å^{-1} calculated using the GFHF $\epsilon(k)$ and using the free particle $\epsilon^0(k)$. Firstly, the position of $\chi^0(Q,E)$ on the energy axis E is effectively the same in both cases. This tells us that the "effective mass" associated with Re$\epsilon(k)$ is indeed $m^*\approx 1$. Secondly, the chief difference is that the χ^0 calculated with the GFHF $\epsilon(k)$ is reduced in intensity at the peak and is spread over a wider energy range due to the imaginary part of $\epsilon(k)$. Otherwise, the two χ^0 are very similar.

In Fig. 3 we show the $S^0(Q,E)$ for $Q=2$ Å^{-1} given by (9), calculated using a purely free-particle energy spectrum, $\epsilon^0(k)=\hbar^2k^2/2m^*$, for three arbitrary choices of the effective mass m^*. The purpose of Fig. 3 is to demonstrate that by simply adjusting the effective mass m^* it is not possible to find an $S^0(Q,E)$ to fit the observed data of Sköld and Pelizzari.[4] Even at high Q ($Q\gtrsim 2$ Å^{-1}), an interparticle interaction is clearly evident in the observed $S(Q,E)$. A qp-qh interaction Γ is needed in (8) to change the shape of $S(Q,E)$ from $S^0(Q,E)$ to the shape observed.

Figure 4 shows the GF T-matrix interaction $\Gamma(Q,E)$ at $Q=2$ and 5 Å^{-1} as a function of energy E. There we notice that the spin-antisymmetric interaction Γ^a is small, both in terms of the real and imaginary parts. This means that the spin-dependent $S_I(Q,E)$ will differ little from $S_0(Q,E)$. The spin-symmetric $\Gamma^s(Q,E)$, however, is large

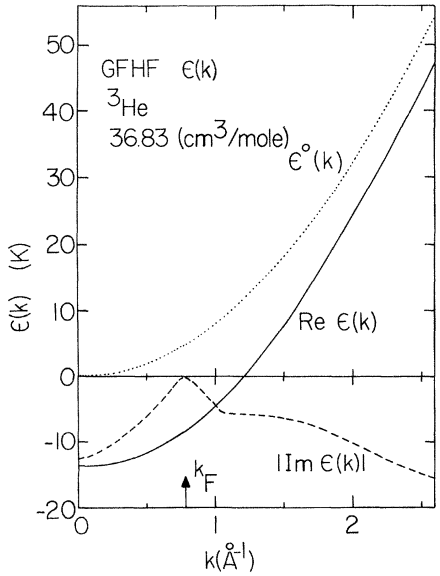

FIG. 1. GFHF single-particle energy spectrum $\epsilon(k)$ in liquid ^{3}He; $\epsilon^0(k)=\hbar^2k^2/2M$.

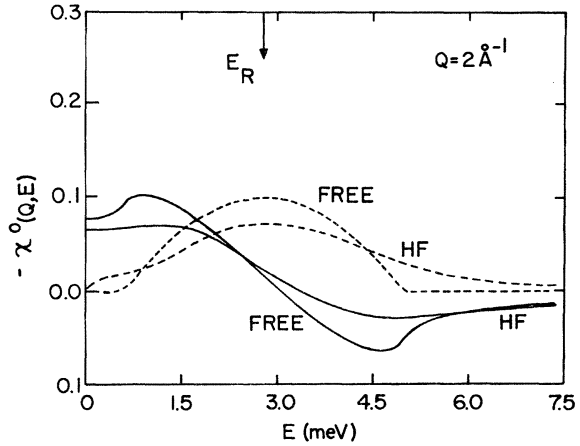

FIG. 2. Dynamic susceptibility χ^0 (——, Reχ^0; — — —, Imχ^0) for noninteracting fermions (3) calculated using both free (FREE) particle energies $\epsilon^0(k)=\hbar^2k^2/2M$ and the GFHF single-particle energies (HF). χ_0 is divided by $dn/d\epsilon=m^*k_F/(\pi^2\hbar^2)$, the density of states per unit volume at ϵ_F^* using $m^*=3.1M$. E_R is the free-particle recoil energy.

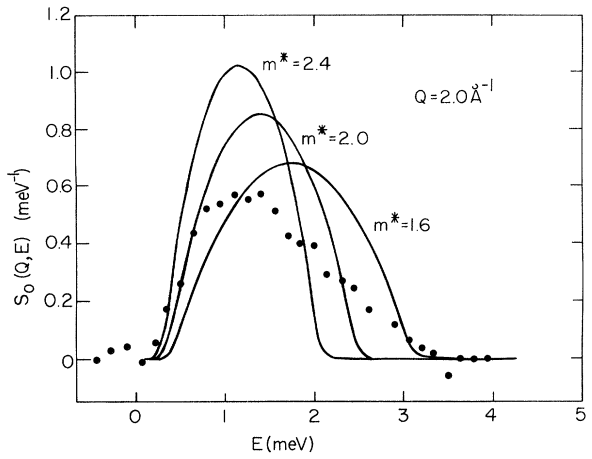

FIG. 3. $S_0(Q,E)$ for a noninteracting Fermi gas having variable effective mass m^* at volume 36.83 cm^3/mole.

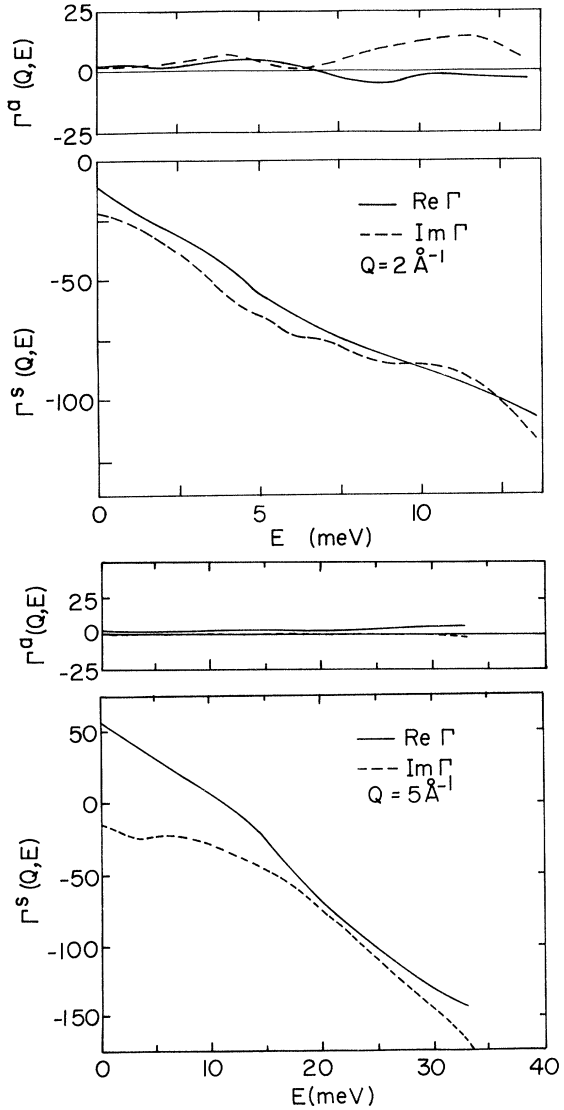

FIG. 4. GF T-matrix:spin-symmetric, $\Gamma^s(Q,E)$, and spin-antisymmetric, $\Gamma^a(Q,E)$, interactions at $Q=2$ and 5 Å^{-1}. Γ is shown multiplied by $dn/d\epsilon=m^*k_F/\pi^2\hbar^2=0.015$ (K Å^3)$^{-1}$, and is therefore in the same dimensionless scale as the Landau parameters.

and negative. Since a negative interaction shifts $\mathrm{Im}\chi(Q,E)$ in (2) toward lower energies E, we expect $S_c(Q,E)$ to peak at a lower energy than $S_0(Q,E)$.

In Fig. 5 we show the $S_c(Q,E)$ and $S_I(Q,E)$ calculated from (8) and the general relation (1) at $T=0$ K, and the total $S(Q,E)$ given by (4). As expected, S_I differs little

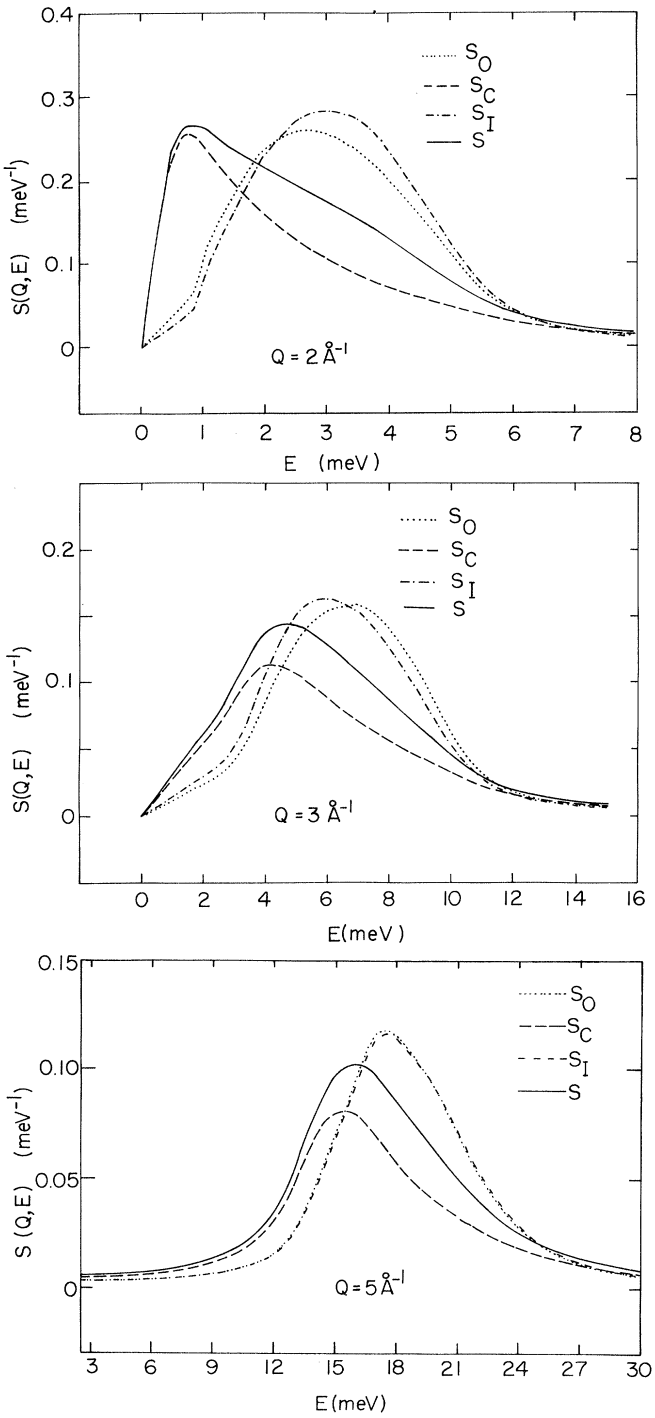

FIG. 5. Coherent, $S_c(Q,E)$, spin-dependent, $S_I(Q,E)$, and total dynamic form factor, $S(Q,E)=S_c(Q,E)+\sigma_i/\sigma_c S_I(Q,E)$, calculated for liquid ^{3}He at volume 36.83 cm^3/mole and $T=0$ K using the T-matrix interaction. $S_0(Q,E)$ is given by (9) using the GFHF energies $\epsilon(k)$ in (3).

from $S_0(Q,E)$ because Γ^a is small. Also, S_c is indeed shifted to lower E due to the negative value of $\mathrm{Re}\Gamma^s$. The $\mathrm{Im}\Gamma^s$ serves to lower the intensity in the peak region of $S_c(Q,E)$ and extend it to higher E values. The impact of Γ^s on S_c is reduced somewhat at the higher Q values.

In the upper half of Fig. 6 we compare the total $S(Q,E)$ calculated from (4) with the observed values of $S(Q,E)$ obtained by Sköld and Pelizzari. In this comparison there are no free parameters and the measurements provide an unadjusted value of $S(Q,E)$ in meV^{-1}. From the upper part of Fig. 6 we see that the calculated intensity is too small by a factor of 2 in the peak region, and the calculated $S(Q,E)$ reaches up to higher energies than is observed. However, an interaction of approximately the magnitude of $z_k^2\,\mathrm{Re}\Gamma^s(Q,E)$ is clearly needed to shift $S(Q,E)$ into the energy range needed for agreement with experiment. In the lower half of Fig. 6 we show the $S(Q,E)$ obtained by setting the imaginary part of the interaction equal to zero, $\mathrm{Im}\Gamma^s(Q,E)=0$. This agrees very well both in magnitude and in energy scale with the observed $S(Q,E)$. This suggests that the $z_k^2\,\mathrm{Im}\Gamma^s$ given by the T matrix is too large, but that the real part of Γ^s has both the correct sign and magnitude.

In Fig. 7 we compare our calculated $S(Q,E)$ with the scattered intensity observed by Stirling *et al.*[2] at a constant scattering angle of 84°. In a constant-angle measurement, Q varies somewhat with energy transfer as shown at the top of Fig. 7. The observed intensity is also determined within an unknown constant only, so that the calculated $S(Q,E)$ can be adjusted relative to the observed intensity by a single overall constant. In the upper half of Fig. 7 we see that the calculated $S(Q,E)$ fits reasonably well, but is broader than the observed intensity. While a constant-Q scan is somewhat broader than a constant-angle scan, the calculated $S(Q,E)$ is definitely broader than the observed intensity would be if converted to a constant-Q mode. Also, $S(Q,E)$ peaks at a somewhat lower energy than the observed intensity. In the lower half of Fig. 7 we see the $S(Q,E)$ calculated with the imaginary part of the T matrix set to zero agrees extremely well with the observed intensity. Again, this suggests that the real part of the T matrix represents the p-h interaction well, but that the imaginary part is too large.

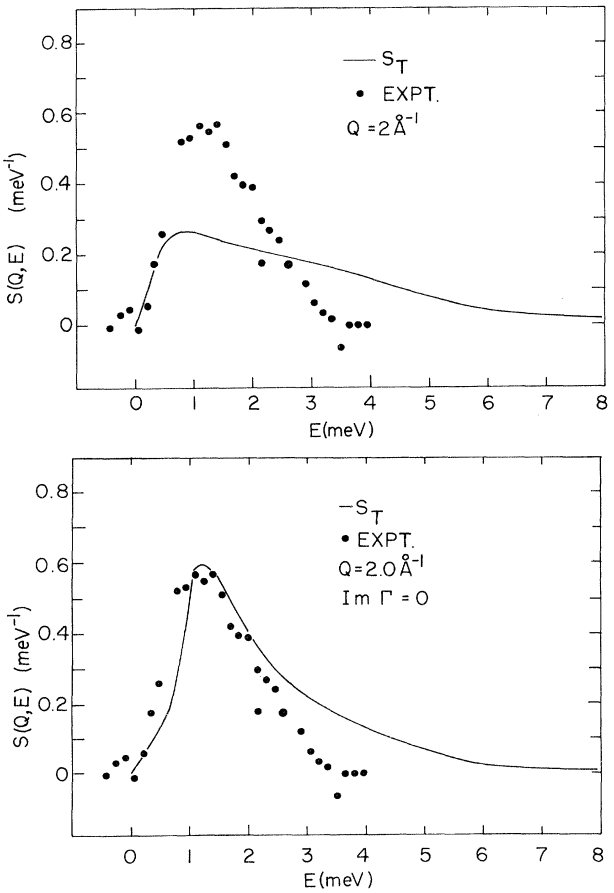

FIG. 6. $S(Q,E)$ calculated using the GF T-matrix interaction and GFHF single-particle energies: upper half, the full T matrix is retained; lower half, the imaginary part of the T matrix is set to zero. The points are the observed values of Sköld and Pelizzari (Ref. 4).

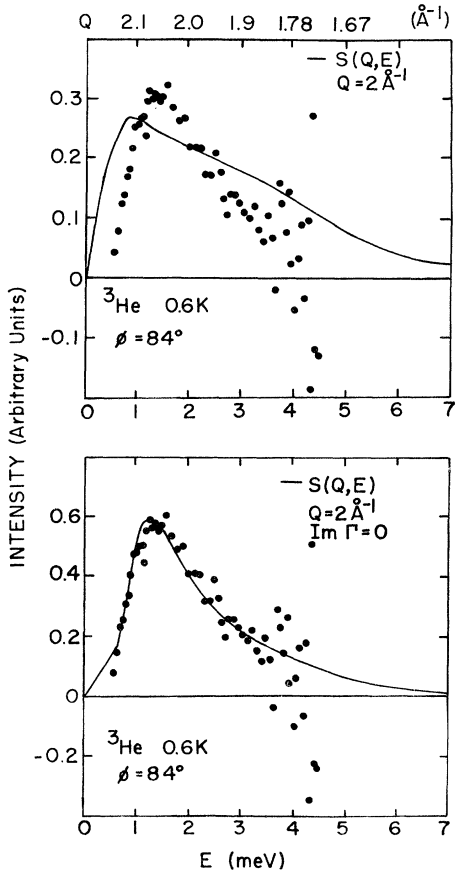

FIG. 7. $S(Q,E)$, as in Fig. 6, compared with the scattering intensity observed by Stirling *et al.* (Ref. 2) at constant scattering angle $\phi=84°$. The corresponding Q value for this ϕ is shown as a function of E at the top of the graph.

IV. DISCUSSION

From Fig. 5 we see the coherent $S_c(Q,E)$ calculated with the GF T-matrix interaction peaks at a lower energy than the noninteracting $S_0(Q,E)$. Since $S_c(Q,E)$ dominates the total $S(Q,E)$, the total $S(Q,E)$ also peaks at a

lower energy than $S_0(Q,E)$. At $Q \approx 2$ Å^{-1}, where there is data for comparison, Figs. 6 and 7 show that this peaking at lower energy is needed to obtain agreement with experiment. In an RPA-like theory at least, a negative interaction (Γ) makes $S(Q,E)$ peak at a lower energy, while a positive interaction pushes $S(Q,E)$ up to higher energy. The comparison with experiment in Figs. 6 and 7 therefore broadly confirms that $\Gamma^s(Q,E)$ should be negative, as shown in Fig. 4, and of approximately the magnitude $z_k^2\Gamma^s(Q,E)$ given by the GF T matrix.

The $z_k^2\Gamma^a(Q,E)$, on the other hand, is so small that $S_I(Q,E)$ differs little from the noninteracting $S_0(Q,E)$. Since it is impossible at present to isolate $S_I(Q,E)$ from the total observed $S(Q,E)$, it is not possible to confirm or refute whether the T-matrix approximation to $z_k^2\Gamma^a(Q,E)$ is approximately correct or not. However, if $\Gamma^a = \frac{1}{2}(\Gamma^{\uparrow\uparrow} - \Gamma^{\uparrow\downarrow})$ is indeed small in the range $2 < Q < 5$ Å^{-1}, then this suggests that the interaction is dominated by the hard core of the potential, with Fermi statistical repulsion arising from the Pauli principle (in $\Gamma^{\uparrow\uparrow}$, but not in $\Gamma^{\uparrow\downarrow}$) playing a relatively minor role.

In the range $2 < Q < 5$ Å^{-1}, the observed $S(Q,E)$ in liquid ^{4}He (Refs. 27 and 28) and in solid ^{4}He (Refs. 29 and 30) also peaks below that expected for scattering from free particles, i.e., below the recoil energy $E_R = \hbar^2Q^2/2M$. This suggests that there is something common in the interaction between the helium atoms in all these systems independent of the statistics and the phase. That is, the difference in statistics between liquid ^{3}He and ^{4}He apparently does not play a major role, as has been proposed at all Q by Pines,[15] nor does any difference in the collective excitations between the solid and the liquid apparently have a major impact on the interaction in this energy and momentum range. The common feature is, of course, the bare potential, and the total interaction is therefore apparently dominated by the "direct" component via the bare potential at large energy transfers. This component should be well approximated by a T matrix in this momentum range. The chief disagreement with experiment is that the calculated $S(Q,E)$ is too broad, indicating that the imaginary part of the T matrix [and possibly of $\epsilon(k)$] is too large.

In Fig. 8 we show the "on-energy-shell" GF T matrix, $\Gamma^s(k,E)$, where $k = \frac{1}{2}(k_1 - k_2) = \frac{1}{2}Q$ is the relative incoming momentum of the two particles, and $E = \epsilon(k_1) + \epsilon(k_2)$ is the on energy shell [with the c.m. momentum $P = 0$, $E = 2\epsilon(k)$]. Also shown in Fig. 8 are the effective interactions determined empirically by Aldrich and Pines,[6] by Glyde and Khanna,[8] and the interaction calculated by Krotscheck,[31] using the method of correlated basis functions (CBF's). These latter effective interactions are selected expressly for use in an RPA-like form (2) to calculate $S(Q,E)$ or the static structure factor $S(Q)$ with emphasis on accuracy at low Q. Indeed, the interaction $U(Q)$ by Krotscheck is obtained by calculating $S(Q)$ using the CBF method and determining $U(Q)$ from $U(Q) = (E_R/2)[S^{-2}(Q) - S_0^{-2}(Q)]$. The Aldrich and Pines interaction is determined in a similar spirit from the difference between the observed $S(Q)$ and the noninteracting Fermi gas $S_0(Q)$. The Glyde and Khanna interaction was determined by using the observed Landau

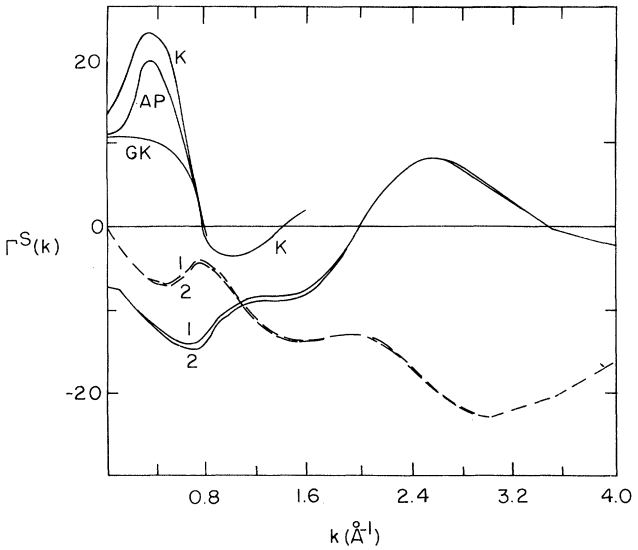

FIG. 8. On-energy-shell spin-symmetric GF T matrix, $\Gamma^s[k,\epsilon(k)]$: (1) Beck potential (Ref. 25) and (2) HFDHE2 potential (Ref. 26) (——, ReΓ^s; — — —, ImΓ^s). The static part of (a) the empirically determined potentials of Aldrich and Pines (AP and of Glyde and Khanna GK), and (b) the potential calculated by Krotscheck (K) using the CBF method is also shown. Here, $k = Q/2$.

parameter F_0^s (at $Q = 0$) and invoking sum-rule arguments. These interactions correspond to the high-frequency limit of the full interaction including induced contributions (the Γ^ω discussed by Abrikosov *et al.*[32]) and should be valid at low Q. At $Q \geq 2.5$ Å^{-1}, where $S(Q) = S_0(Q) = 1$, the $U(Q)$ defined above must vanish.

On the other hand, we expect the T matrix to represent the full interaction in (2) at high Q, but to be inappropriate in (2) at low Q, where induced contributions dominate. The T matrix is the interaction which enters the GFHF ground-state energy and must remain negative at low Q in order to obtain a bound liquid. It is not the same effective interaction as the AP polarization potentials or the $U(Q)$, and was not designed for use in (2). It does not, for example, contain induced interactions and is not the high-frequency limit of the full interaction. However, at sufficiently high Q we expect induced interactions to be relatively unimportant, and expect all effective interactions to reduce approximately to the T matrix. From Fig. 4 this T-matrix interaction is still highly energy dependent. In this sense, the T matrix and earlier interactions complement each other, and are valid in different momentum-transfer ranges.

Finally, use of the form (2), with a T-matrix interaction and a Hartree-Fock $\epsilon(k)$, essentially excludes any scattering from multiparticle-hole excitations. While the neutron creates single p-h excitations, coupling to multiparticle-hole (mp-h) excitations via the p-h interaction is possible. We find the present $S_c(Q,E)$ takes up approximately 85% of the f sum rule independent of Q in the range $2 \leq Q \leq 5$ Å^{-1}. This suggests that the mp-h component, neglected here, accounts for approximately 15% of the total $S_c(Q,E)$. This is consistent with the cal-

culations of Aldrich and Pines,[6] and of Sköld and Pelizzari[4] at lower Q. On the other hand, the $S_I(Q,E)$ and $S_0(Q,E)$ exceed the f sum rule by approximately 10%, when the GFHF $\epsilon(k)$ spectrum is used. An improved theory should include mp-h excitations, although this is unlikely to improve agreement with experiment in the present case. It would also be interesting to see whether including induced interactions would reduce ImΓ.

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